

Vapor Pressures, Critical Parameters, Boiling Points, and Triple Points of Ammonia and Trideuteroammonia

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A simple extended corresponding-states principle is used to represent the vapor pressure of ammonia and trideuteroammonia from the triple point to critical point and to describe the available experimental data along with extrapolation beyond their ranges of available experimental data. This work takes advantage of the adoption of the ITS-90 temperature scale and of the new critical parameters obtained from the extended corresponding-states principle. The vapor pressure data are described within their scatter in the entire temperature range. Comparisons with the available data show that the extended corresponding-states principle may calculate the vapor-pressure values within 0.05%–0.1%. The substance-dependent characteristic parameters are given, such as critical temperature, critical density, critical pressure, acentric factor, and aspherical factor. The values of the pressures, along with their first and second derivatives as a function of temperature over the entire region from the triple point to the critical point are tabulated and recommended for scientific and practical uses. © 2004 American Institute of Physics. [DOI: 10.1063/1.1691451]

Key words: ammonia; boiling point; corresponding-states principle; critical density; critical parameters; critical pressure; critical temperature; ITS-90; thermodynamic properties; trideuteroammonia; triple point; vapor pressure.

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1. Introduction

Reliable data on the thermophysical properties of ammonia (NH_3) and trideuteroammonia (ND_3) are required for many practical applications. Since the available experimental information on the thermophysical properties of ammonia is limited, a prediction technique must be made with the aid of various theoretical methods such as the corresponding-states principle. Baehr *et al.*¹ in 1976 and Haar and Gallagher² in 1978 published correlations for vapor pressure from the triple point to the critical point for ammonia respectively. Tillner-Roth *et al.*³ published a fundamental equation of state from which the vapor pressure may be calculated with some inconveniences in 1993. No vapor-pressure equation was proposed for trideuteroammonia from the triple point to the critical point.

For the description of a vapor pressure equation for ammonia, two subsequent advances are pertinent:

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- (1) A new representation of the thermodynamic temperature scale, known as ITS-90 (Preston-Thomas⁴); and
- (2) A simple extended corresponding-states principle that can be applied to highly nonspherical substances, as was recently developed by Xiang.⁵⁻⁸

This corresponding-states approach was shown to be applicable to all substances and it is applied here to ammonia.

2. Present Method

2.1. Vapor-Pressure Equation

To represent experimental data over the entire range from the triple point to the critical temperature, the vapor-pressure curve was based upon an equation with known physical behavior and has only three substance-dependent parameters as described in the Xiang–Tan equation,⁹

$$\ln p_r = (a_0 + a_1 \tau^{n_1} + a_2 \tau^{n_2}) \ln T_r, \quad (1)$$

where $\tau = 1 - T_r$, the reduced temperature $T_r = T/T_c$ with T_c being the critical temperature, and $p_r = p/p_c$ with p_c being the critical pressure. The value of n_1 is 1.89 and the values of n_2 is $3n_1$ or 5.67. The substance-dependent parameter a_0 is the Riedel parameter¹⁰ and a_1 and a_2 are substance-dependent parameters. The functional form presented in Eq. (1) is rewritten as

$$p_r = \exp[(a_0 + a_1 \tau^{n_1} + a_2 \tau^{n_2}) \ln T_r] \quad (2)$$

and

$$p = p_c \exp[(a_0 + a_1 \tau^{n_1} + a_2 \tau^{n_2}) \ln T_r]. \quad (3)$$

The slope of the vapor-pressure equation is given by

$$dp/dT = \frac{d \ln p_r}{dT_r} p/T_c, \quad (4)$$

where

$$\begin{aligned} \frac{d \ln p_r}{dT_r} &= (a_0 + a_1 \tau^{n_1} + a_2 \tau^{n_2})/T_r \\ &\quad - (n_1 a_1 \tau^{n_1-1} + n_2 a_2 \tau^{n_2-1}) \ln T_r. \end{aligned} \quad (5)$$

At the critical point, $d \ln p/d \ln T = \alpha_c$ is the Riedel parameter.¹⁰

The second derivative of pressure as a function of temperature is given by

$$d^2 p/dT^2 = \left[\frac{d^2 \ln p_r}{dT_r^2} + \left(\frac{d \ln p_r}{dT_r} \right)^2 \right] p/T_c^2, \quad (6)$$

where

$$\begin{aligned} \frac{d^2 \ln p_r}{dT_r^2} &= [n_1(n_1-1)a_1 \tau^{n_1-2} + n_2(n_2-1)a_2 \tau^{n_2-2}] \ln T_r \\ &\quad - (a_0 + a_1 \tau^{n_1} + a_2 \tau^{n_2})/T_r^2 \\ &\quad - 2(n_1 a_1 \tau^{n_1-1} + n_2 a_2 \tau^{n_2-1})/T_r. \end{aligned} \quad (7)$$

Equation (1) can be used to extrapolate from the precise vapor pressure measurements at modest pressures to the criti-

TABLE 1. General coefficients of the extended corresponding-states principle for vapor pressure in Eq. (9)

a_{00}	5.790206	a_{10}	6.251894	a_{20}	11.65859
a_{01}	4.888195	a_{11}	15.08591	a_{21}	46.78273
a_{02}	33.91196	a_{12}	-315.0248	a_{22}	-1672.179

cal point and to the triple point, provided that the critical temperature is known. When the temperature approaches the critical point, the second derivative should weakly approach infinity, which becomes significant only near several thousandth of τ . For this case, the amplitude of the leading-order nonanalytic term in Eq. (6) is not consistent with the correct universal amplitude.

2.2. The Extended Corresponding-States Principle

The two-parameter corresponding-states method can only be applied accurately to spherical molecules, e.g., argon, krypton, and xenon. In order to extend the corresponding-states principle to molecular fluids, it is necessary to take into account the non-spherical nature of real molecules through the acentric factor defined by Pitzer *et al.*,¹¹ which works well for a wide range of nonpolar substances but its predictive capability for polar and associating molecules is generally poor. The use of four parameters for polar fluids corresponds to an intermolecular potential function in which dispersion and dipole–dipole interaction effects are accounted for. To extend the corresponding-states principle of Pitzer *et al.*¹¹ to highly nonspherical substances, the recently developed extended corresponding-states parameter, $\theta = (Z_c - 0.29)^2$, was introduced to describe the deviation of the critical compression factor, Z_c , of a real nonspherical molecule from spherical molecules.⁵⁻⁸ For spherical fluids $Z_c = 0.29$. The aspherical factor θ is obtained from the parameters of the behavior in the critical state, which are effected by the dipole and quadrupole moments. The aspherical factor θ reflects the physical behavior displayed by the dipole and quadrupole moments and may measure the behavior of the deviation of a highly nonspherical molecule from that of the spherical molecule argon, as is similar to the definition of the acentric factor. The relation between the critical compression factor and acentric factor, $Z_c = 0.29 - 0.08\omega$,^{11,12} is only approximate for nonpolar substances and is not applicable to highly nonspherical substances. It should be noted that the aspherical factor θ is independent for a real molecule, which significantly improves the corresponding-states behavior of polar substances. It may be deduced that the extended corresponding-states principle corresponds to adding a quadratic term $0.0064\omega^2$ to the theory of Pitzer *et al.*¹¹ for normal fluids.

The extended corresponding-states principle for vapor pressure reads as follows:

$$\ln p_r = \ln p_r^{(0)} + \omega \ln p_r^{(1)} + \theta \ln p_r^{(2)}, \quad (8)$$

where the acentric factor,¹¹ $\omega = -1 - \log p_r|_{T_r=0.7}$ and the aspherical factor,⁵⁻⁸ $\theta = (Z_c - 0.29)^2$ are corresponding-states

TABLE 2. Experimental vapor-pressure data sources for ammonia and trideuteroammonia

Author(s)	Year	Data points	Temperature range (K)	Pressure range (kPa)	ΔT (K)	Δp (kPa)
Ammonia						
Baehr <i>et al.</i> ¹	1976	16	328–403	2325–10973	0.008	0.1(1.7 + p)
Beattie and Lawrence ²¹	1930	14	303–405	1166–11298		0.2%
Brill ¹⁴	1906	20	193–243	4.69–101.3		
Burrell and Robertson ¹⁵	1915	17	159–238	0.133–101.3		
Cragoe <i>et al.</i> ¹⁶	1920	150	195.4–343	5.98–3312	0.01	0.02%–0.05%
Date ²³	1973	9	298–405	1011–11302		
Gillespie <i>et al.</i> ²⁵	1987	4	313–394	1565–9266	0.03	0.3%
Henning and Stock ¹⁹	1921	5	196.6–243	6.75–118.8		
Holcomb and Outcalt ²⁷	1999	14	280–389	558–8542	0.05	3.5
Ichihara and Uematsu ²⁶	1994	12	310–400	1423–10304	0.01	0.03%
Keyes and Brownlee ¹⁸	1918	70	273–398	435.6–9957		0.3%
Overstreet and Giauque ²²	1937	17	195.4–241	6.075–111.3	0.05	0.00133
Zander and Thomas ²⁴	1979	33	293–392	8686–9015	0.01	0.005%
Trideuteroammonia						
Taylor and Jungers ²⁸	1934	5	202–238	8.3–83.7		
Jungers and Taylor ²⁹	1934	5	202–238	8.3–83.7		
Calado <i>et al.</i> ³⁷	1992	62	228–259	48.2–222	0.01	
Groth <i>et al.</i> ³²	1956	31	273–294	399–835		
Hart and Partington ³¹	1943	15	212–243	17.8–106.5		
King <i>et al.</i> ³⁶	1989	6	198.5–243	6.22–105.5	0.001	0.005%
Kirshenbaum and Urey ³⁰	1942	23	202–235	8.3–72.7		
Streatfeild <i>et al.</i> ³⁵	1987	13	200–265	7.58–295	0.01	0.1%
Wolff and Hoepfner ³⁴	1969	13	218–273	25.3–396		

parameters, here $Z_c = p_c / R \rho_c T_c$ is the critical compression factor and $R = 8.314\,472\text{ J K}^{-1}\text{ mol}^{-1}$ is the molar gas constant recommended by Mohr and Tayler.¹³

To predict the vapor pressure from the corresponding-states principle, the proper reference equation must be selected which is valid from the triple point to the critical point. Equation (1) fulfills this requirement in that it can be used effectively to correlate and extrapolate the vapor-pressure behavior of simple, nonpolar, polar, hydrogen-bonding, and associating compounds. Therefore, the corresponding-states method can be used to represent vapor pressures over the entire range as^{5–8}

$$\begin{aligned}\ln p_r^{(0)} &= (a_{00} + a_{10}\tau^{n_1} + a_{20}\tau^{n_2}) \ln T_r, \\ \ln p_r^{(1)} &= (a_{01} + a_{11}\tau^{n_1} + a_{21}\tau^{n_2}) \ln T_r, \\ \ln p_r^{(2)} &= (a_{02} + a_{12}\tau^{n_1} + a_{22}\tau^{n_2}) \ln T_r.\end{aligned}\quad (9)$$

The general coefficients a_{ij} of Eq. (9), given in Table I, were found from fitting the vapor-pressure data for argon, the weakly nonspherical molecules ethane, propane, difluoroethane, 1,1,1,2-tetrafluoroethane, 1,1-difluoroethane, and the highly nonspherical molecule water. The coefficients are independent of the specific substance and are expected to be universal for all classes of molecules.^{5–8}

3. Experimental Vapor-Pressure Data from the Literature

Brill¹⁴ determined the vapor pressure of ammonia between 193.15 K and 240 K.

Burrell and Robertson¹⁵ measured the vapor pressure of ammonia from 159.8 K to 238.5 K.

Cragoe *et al.*¹⁶ measured the vapor pressure of ammonia in the temperature from 195.4 K to 343 K over which temperature range 150 data points were taken in the first of two experiments, including 11 determinations for the normal boiling point. The data were taken at near uniform intervals except near the values of temperature associated with important fixed points, for which data were taken over very small intervals. Results for the boiling point were verified by a second set of measurements based on a completely independent experimental procedure. Values of temperature were measured with platinum resistance thermometers. Pressures were measured with mercury manometers and a piston gauge. The scatter of the data was in large part associated with the precision of the pressure measurements, which was about 1 part in 5000 for pressure above several atmospheres. The experimental method used for the main body of data is referred to as the static method. Certain modifications were required below 218.15 K for which region measurements were made for only three values of temperature. Throughout, the experimental values of temperature were believed to within 0.01 K. The second set of measurements was limited to determination of the normal boiling point. These measurements were based on an experimental procedure referred to as the dynamic method, which is comparatively insensitive to the presence of impurities or to the attainment of equilibrium. The mean of 17 dynamic measurements agreed with results for the determinations by the static method to within about 0.01 K and the authors suggested a value for the boil-

TABLE 3. Critical parameters for ammonia and trideuteroammonia

Author(s)	Year	Critical temp. (K)	Critical pressure (kPa)	Critical density ($\rho_c/\text{kg m}^{-3}$)
Ammonia				
Dewar ³⁸	1884	403.15	11652	
Vincent and Chappins ³⁹	1886	404.15	11450	
Centnerswer ⁴⁰	1903	405.68		
Mathias ⁴¹	1904			239
Jacquero ⁴²	1908	405.45		
Scheffer ⁴³	1910	405.25	11277	
Cardoso and Giltay ⁴⁴	1912	406.05	11379	
Berthoud ⁴⁵	1918	405.45		236
Postma ⁴⁶	1920	405.5	11277	
Cragoe <i>et al.</i> ⁴⁷	1922			234
Date ⁴⁸	1973	405.417	11318	236
Baehr ¹	1976	405.367	11353	234
Haar and Gallagher ²	1978	405.367	11336	235
Kiselev and Rainwater ⁴⁹	1997	405.036	11277	234
Edison and Sengers ⁵⁰	1999	405.367	11336	235
This work		405.37	11345	234.3
Trideuteroammonia				
Kopper ⁵¹	1992	405.2		
This work		405.2	11300	276

ing point of 239.827 K which is the average for the two methods. An overall uncertainty of 0.01 K results in an uncertainty of less than 0.1% in vapor pressure at 233.15 K. With increasing values of temperature, an uncertainty in vapor pressure becomes less than 0.05% at 273.15 K and less than 0.03% at 343.15 K. The pressure measurement indicated an uncertainty of about 0.02% for pressure above several atmospheres.

Keyes¹⁷ reported vapor pressure measurements for values of temperature above 273.15 K, which corrected earlier results of Keyes and Brownlee.¹⁸ The temperature scale employed was very nearly identical to ITS 1927 above 273.15 K. The data reported by Keyes and Brownlee¹⁸ have very large scatter, nearly 0.3% at the higher temperatures. These measurements extend the range of the values reported by Cragoe *et al.*¹⁶ to near the critical temperature. The data ob-

tained by Keyes¹⁷ agree with those of Cragoe *et al.*¹⁶ in their region of overlap with a maximum deviation of 0.06% and an average deviation of 0.03%, which is within the precision of either set of measurements.

Henning and Stock¹⁹ reported measurements in the range from the triple point to 243 K. These data have average deviation from that of Cragoe *et al.*¹⁶ of 0.3%.

McKelvey and Taylor²⁰ measured two triple-point vapor pressures and four triple-point temperatures. The spread in the four temperature measurements was less than 0.01 K with the average value of 195.493 K reported as the value of the triple-point temperature. The two vapor-pressure measurements differed by 27 Pa. The mean of the two, 6.026 kPa, was reported at the triple-point pressure. If the principal uncertainty in the pressure measurements is associated with the precision of the manometer, then a 27 Pa scatter in the data represents nearly a 0.5% error in the measured values for the triple-point pressure. The value reported for the triple-point temperature would appear to be uncertain by no more than about 0.010 K to 0.015 K.

Beattie and Lawrence²¹ measured vapor pressure from 303.15 K to near the critical temperature, using an experimental procedure similar to that employed by Keyes.¹⁷ At the lower temperature, these results are in excellent agreement with those of Cragoe *et al.*¹⁶ within 0.03% at 303.15 K, however, the difference increases slightly with increasing values of temperature to just under 0.1% at 343.15 K, with an average deviation in this range of about 0.05%. The agreement is within their reported uncertainty. Above 343.15 K the data agree with those of Keyes¹⁷ to within 0.1% up to 383.15 K. Differences increase to about 0.2% at 393.15 K and then uniformly to 0.8% at 405.15 K, the highest value of temperature reported, with the values of Beattie and Lawrence²¹ being consistently higher throughout.

Overstreet and Giauque²² measured the vapor pressure from the triple point to 241.6 K. Values of temperature were measured with a special gold resistance-thermometer-heater, but the primary standard was a thermocouple, which was calibrated with a hydrogen gas thermometer and compared from time to time with the gas thermometer. Such a compari-

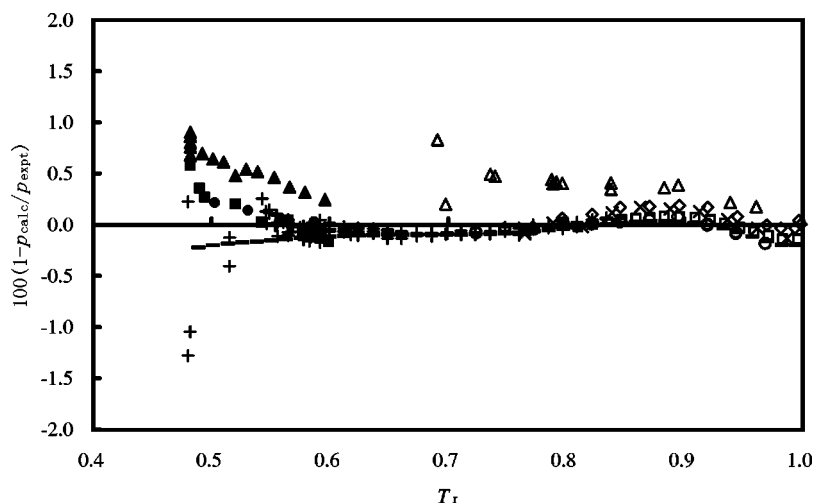


FIG. 1. Comparison of the experimental vapor-pressure data for ammonia with values calculated from the extended corresponding-states principle. (\square) Baehr *et al.*¹ (\diamond) Beattie and Lawrence²¹; (+) Cragoe *et al.*¹⁶; (\bullet) Henning and Stock¹⁹; (\triangle) Holcomb and Outcalt²⁷; (\times) Ichihara and Uematsu²⁶; (\blacktriangle) Overstreet and Giauque²²; (\circ) Zander and Thomas²⁴; (---) Baehr *et al.*¹ (original).

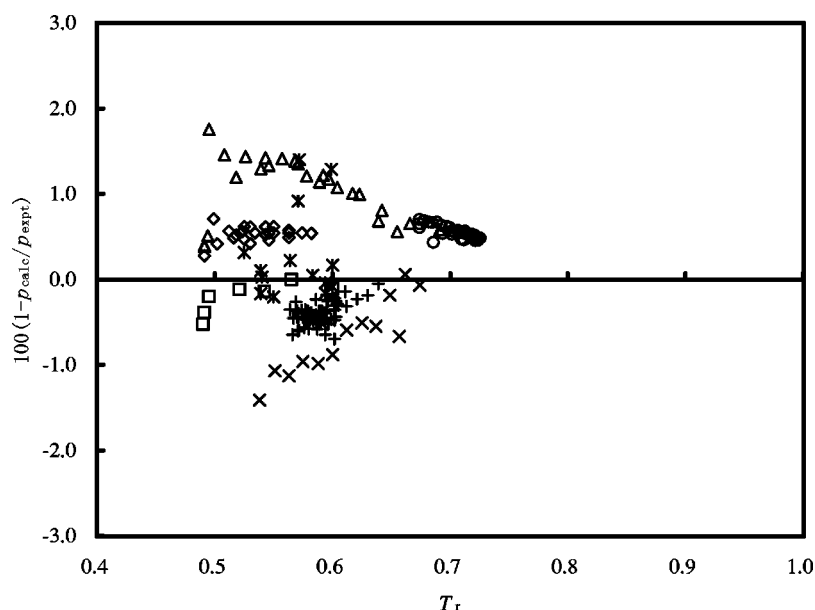


FIG. 2. Comparison of the experimental vapor-pressure data for trideuteroammonia with values calculated from the extended corresponding-states principle. (+) Calado *et al.*³⁷; (O) Groth *et al.*³²; (*) Hart and Partington³¹; (□) King *et al.*³⁶; (◇) Kirshenbaum and Urey³⁰; (Δ) Streatfield *et al.*³⁵; (x) Wolff and Hoefner.³⁴

son was also made immediately following this experiment and the values of temperature measurements were adjusted accordingly. The precision of the gold resistance thermometer was 0.001 K, as compared with 0.01 K to 0.02 K for the primary standard, the thermocouple. Values of Overstreet and Giauque²² are lower than that of Cragoe *et al.*¹⁶ by about 0.04 K and 0.05 K at the triple point and the boiling point, respectively. This difference is consistent with their observations that the temperature scale can be in error by as much as 0.05 K. The pressure measurements were made with a high precision manometer, which could be read to within about 1.33 Pa. The precision achieved for pressure measurements is at least an order of magnitude greater than had been achieved in the earlier work of Cragoe *et al.*¹⁶ The reported vapor-pressure value at the triple point was 6.077 kPa. The value reported by McKelvey and Taylor²⁰ was 6.026 kPa. The difference of 0.05 kPa is outside the combined precision of measurement, and is indicative of a small systematic discrepancy between the two experiments.

Date²³ reported measurements for the vapor pressure for the temperature range from 298.15 K to the critical temperature. The maximum differences occur at 298.15 K for which the results of Date²³ are about 1% too high. At 373.15 K the data reported by Date²³ are too low by about 0.3%. Near the

critical point the measurement by Date²³ tends to average the differences between those of Keyes¹⁷ and of Beattie and Lawrence.²¹

Baehr *et al.*¹ reported a set of very precise data for the vapor pressure from 328.4 K to 403.6 K. These data in their region of overlap are in excellent accord with the result of Cragoe *et al.*¹⁶ to within the scatter of those data. They tend to somewhat lower values than the data of Beattie and Lawrence.²¹ Near the critical point the difference is about 0.1%. The uncertainty of the measured temperature is reported to be 0.008 K. An overall accuracy of these data is 0.05%.

Zander and Thomas²⁴ measured the vapor pressure from 293.5 K to 392.6 K. Values of the vapor pressure obtained from static measurements by using the constant volume apparatus. The reported accuracy of the measured temperature and pressure are 0.01 K and 0.005%, respectively.

Gillespie *et al.*²⁵ reported the vapor pressure of ammonia from 313.15 K to 394.3 K. The accuracy of the measured temperature and pressure are 0.03 K and 0.3%, respectively.

Ichihara and Uematsu²⁶ measured the vapor pressure from 310 K to 400 K. The pressure of the nitrogen gas was measured with two oil-operated dead-weight pressure gauges. These two pressure gauges were calibrated with a precision

TABLE 4. The critical parameters, acentric factor, and aspherical factor for ammonia and trideuteroammonia, which are obtained from the extended corresponding-states principle for vapor pressure given in Eq. (9)

	Ammonia	Trideuteroammonia		Ammonia	Trideuteroammonia
T_c /K	405.37	405.2	a_0	7.115168	7.265948
p_c /kPa	11345	11300	a_1	9.478726	9.904991
ρ_c /kg m ⁻³	234.3	276	a_2	20.236840	21.49400
ω	0.2568	0.287	θ	2.0545×10^{-3}	2.1476×10^{-3}
T_{triple} /K	195.4	199.0	p_{triple} /kPa	6.0182	6.4855
T_b /K	239.79	242.20	M (kg kmol ⁻¹)	17.013	20.05

of 0.03%. The sample pressure was obtained by subtracting the difference between internal and external pressures of the bellows from the pressure of the nitrogen gas. This pressure difference was calibrated with an uncertainty of 0.4 kPa. The accuracy of the measured temperature and pressure is 0.01 K and 0.03%, respectively.

Holcomb and Outcalt²⁷ measured the vapor pressure from 280 K to 389.5 K. The accuracy of the measured temperature and pressure is 0.05 K and 3.5 kPa, respectively.

Taylor and Jungers^{28,29} measured the vapor pressure of trideuteroammonia from 202 K to 238 K.

Kirshenbaum and Urey³⁰ measured the vapor pressure of trideuteroammonia from 202 K to 235 K. The accuracy of the measured temperature is 0.01 K. In the experiment, the triple-point pressures were reproducible to 3 or 4 Pa, an error of 5 Pa may exist in the pressure difference. The average error was estimated as 20 Pa.

Hart and Partington³¹ measured the vapor pressure of trideuteroammonia from 212 K to 243 K with a large scatter of about 1%.

Groth *et al.*³² measured the vapor pressure of trideuteroammonia from 273 K to 294 K.

Kiss *et al.*³³ reported a vapor-pressure equation of trideuteroammonia from 190 K to 243 K without experimental data.

Wolff and Hoepfner³⁴ measured the vapor pressure of trideuteroammonia from 218 K to 273 K.

Streatfeild *et al.*³⁵ measured the difference in the vapor pressure of ammonia and trideuteroammonia between 200 K and 266 K.

King *et al.*³⁶ measured the vapor-pressure differences of ammonia and trideuteroammonia from the triple point to 243 K. The temperature of the isotopic samples contained in separate cavities in a copper block of five-nine purity was controlled with a short-time stability, which was generally far better than 0.001 K and well within 0.001 K of each other. The absolute pressure of ammonia of natural isotopic abundance was measured with a spiral quartz gauge with a resolution of 1 Pa. Measurements of the differences in the isotopic vapor pressures were carried out with a capacitance gauge per isotopic pair.

Calado *et al.*³⁷ measured the vapor pressure between 228 K and 259 K in a twofold differential apparatus using a high-precision manometric technique. The vapor-pressure difference was monitored using capacitance sensors with a resolution of 1.3 Pa. The absolute vapor pressure of trideuteroammonia was simultaneously measured using another capacitance sensor with a resolution of 3.4 Pa. Temperatures were read with a resolution of 0.001 K and an estimated accuracy of 0.01 K.

These data resources are summarized in Table II. As pointed out by Haar and Gallagher,² there exists a considerable spread in the critical values of ammonia represented in the earlier literature as given in Table III. No experimental

TABLE 5. Smoothed pressures, along with their first and second derivatives, as a function of temperature for ammonia

<i>T</i> (K)	<i>p</i> (kPa)	<i>dp/dT</i> (kPa/K)	<i>d²p/dT²</i> (kPa/K ²)	<i>T</i> (K)	<i>p</i> (kPa)	<i>dp/dT</i> (kPa/K)	<i>d²p/dT²</i> (kPa/K ²)
195.40	6.0182	0.4840	3.323E-02	303.15	1167.8	34.70	0.7827
198.15	7.4813	0.5826	3.860E-02	308.15	1351.3	38.76	0.8407
203.15	10.922	0.8031	4.994E-02	313.15	1555.9	43.11	0.9003
208.15	15.616	1.086	6.345E-02	318.15	1782.9	47.76	0.9616
213.15	21.901	1.441	7.928E-02	323.15	2034.0	52.73	1.025
218.15	30.172	1.883	9.756E-02	328.15	2310.7	58.01	1.090
223.15	40.889	2.421	0.1184	333.15	2614.7	63.64	1.159
228.15	54.571	3.071	0.1419	338.15	2947.6	69.60	1.230
233.15	71.805	3.845	0.1680	343.15	3311.3	75.94	1.304
238.15	93.246	4.756	0.1968	348.15	3707.6	82.65	1.383
239.79	101.32	5.087	0.2069	353.15	4138.5	89.78	1.467
243.15	119.61	5.817	0.2283	358.15	4606.1	97.33	1.556
248.15	151.69	7.043	0.2624	363.15	5112.6	105.4	1.653
253.15	190.34	8.446	0.2991	368.15	5660.5	113.9	1.758
258.15	236.47	10.04	0.3382	373.15	6252.3	122.9	1.873
263.15	291.06	11.83	0.3797	378.15	6890.9	132.6	1.998
268.15	355.15	13.84	0.4234	383.15	7579.6	143.0	2.138
273.15	429.82	16.07	0.4693	388.15	8321.7	154.0	2.293
278.15	516.24	18.54	0.5172	393.15	9121.2	165.9	2.467
283.15	615.58	21.24	0.5669	398.15	9982.4	178.7	2.663
288.15	729.11	24.21	0.6184	403.15	10910	192.6	2.889
293.15	858.09	27.43	0.6716	405.37	11345	199.1	3.004
298.15	1003.9	30.93	0.7263				

data in the high-temperature region and for the critical pressure and critical density of trideuteroammonia have been reported yet. All literature data were converted to ITS-90, the temperature scale used throughout this work.

TABLE 6. Smoothed pressures, along with their first and second derivatives, as a function of temperature for trideuteroammonia

<i>T</i> (K)	<i>p</i> (kPa)	<i>dp/dT</i> (kPa/K)	<i>d²p/dT²</i> (kPa/K ²)	<i>T</i> (K)	<i>p</i> (kPa)	<i>dp/dT</i> (kPa/K)	<i>d²p/dT²</i> (kPa/K ²)
199.00	6.4855	0.5180	3.532E-02	303.15	1107.3	33.75	0.7846
203.15	8.9636	0.6824	4.413E-02	308.15	1286.1	37.82	0.8452
208.15	12.977	0.9335	5.671E-02	313.15	1486.0	42.20	0.9076
213.15	18.413	1.253	7.161E-02	318.15	1708.6	46.90	0.9721
218.15	25.645	1.654	8.900E-02	323.15	1955.5	51.93	1.039
223.15	35.107	2.148	0.1090	328.15	2228.4	57.29	1.108
228.15	47.299	2.748	0.1317	333.15	2529.0	63.01	1.179
233.15	62.791	3.469	0.1572	338.15	2859.1	69.09	1.255
238.15	82.218	4.325	0.1855	343.15	3220.6	75.56	1.333
242.20	101.32	5.127	0.2106	348.15	3615.4	82.43	1.417
243.15	106.29	5.330	0.2167	353.15	4045.6	89.73	1.505
248.15	135.79	6.497	0.2507	358.15	4513.5	97.50	1.600
253.15	171.55	7.841	0.2874	363.15	5021.4	105.8	1.703
258.15	214.51	9.375	0.3268	368.15	5571.9	114.5	1.814
263.15	265.64	11.11	0.3688	373.15	6167.8	123.9	1.936
268.15	326.00	13.07	0.4133	378.15	6812.0	133.9	2.070
273.15	396.69	15.25	0.4601	383.15	7508.1	144.6	2.218
278.15	478.90	17.67	0.5092	388.15	8259.6	156.1	2.383
283.15	573.83	20.35	0.5605	393.15	9070.8	168.5	2.568
288.15	682.79	23.28	0.6137	398.15	9946.2	181.8	2.778
293.15	807.08	26.49	0.6688	403.15	10891	196.3	3.019
298.15	948.11	29.97	0.7258	405.2	11300	202.6	3.133

4. Comparisons and Results

The experimental data are compared with values calculated from the present method as shown in Figs. 1 and 2. Additional experimental data in the high temperature region is needed for trideuteroammonia. The critical parameters, acentric factor, aspherical factor, normal-boiling-point and triple-point temperatures are listed in Table IV. Smoothed pressures, along with their first and second derivatives, as a function of temperature in the range between the triple point and the critical point for ammonia and trideuteroammonia from the present method are presented in Tables V and VI.

5. Model Uncertainty

Generally speaking, the uncertainty of vapor pressures determined by the extended corresponding-states method is within the experimental uncertainties for the most accurate data (refer to the extensive application of the present method in previous works^{5–8}). The average deviations between the vapor pressures obtained from the present method, Eq. (9), and the experimental data are shown in Figs. 1 and 2. The uncertainties of the present method were verified to be approximately 0.05%–0.1% in the vapor pressure for substances whose have accurate experimental data, even in a limited range. The uncertainties are less than 0.1% for the first derivative and are several percentages for the second derivative according to our mathematical experience.

6. Conclusions

All data included in the previous vapor pressure equation were converted to the ITS-90 temperature scale. The vapor-pressure values obtained by the extended corresponding-states principle are in agreement with the published experimental data within their uncertainties. The uncertainty in the vapor pressure is estimated at 0.05%–0.1% since the extended corresponding-states principle is used in the present method. The previous vapor-pressure equations for ammonia and trideuteroammonia do not adequately describe these data because it was based on the IPTS-68 temperature scale and in a limited range. An advantage of the present method is that it allows accurate values to be calculated directly without requiring any temperature conversion.

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